Supporting Information

Structure and Properties of Boron-Very-Rich Boron Carbides: B_{12} Icosahedra Linked through Bent CBB Chains

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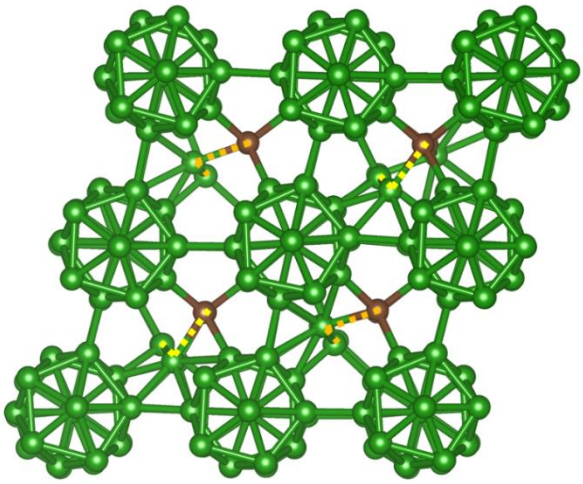

Fig. S1 The optimized (B_{12})CBB structure transformed from linear chain structure after AIMD simulations. The CBB chain bends to two different directions, labeled with yellow color dot line and orange color dot line. The lattice parameters are: a = 10.384 Å, b = 10.238 Å, c = 10.232 Å, α = 67.9°, β = 66.5°, and γ = 66.3°.